

Figure 1

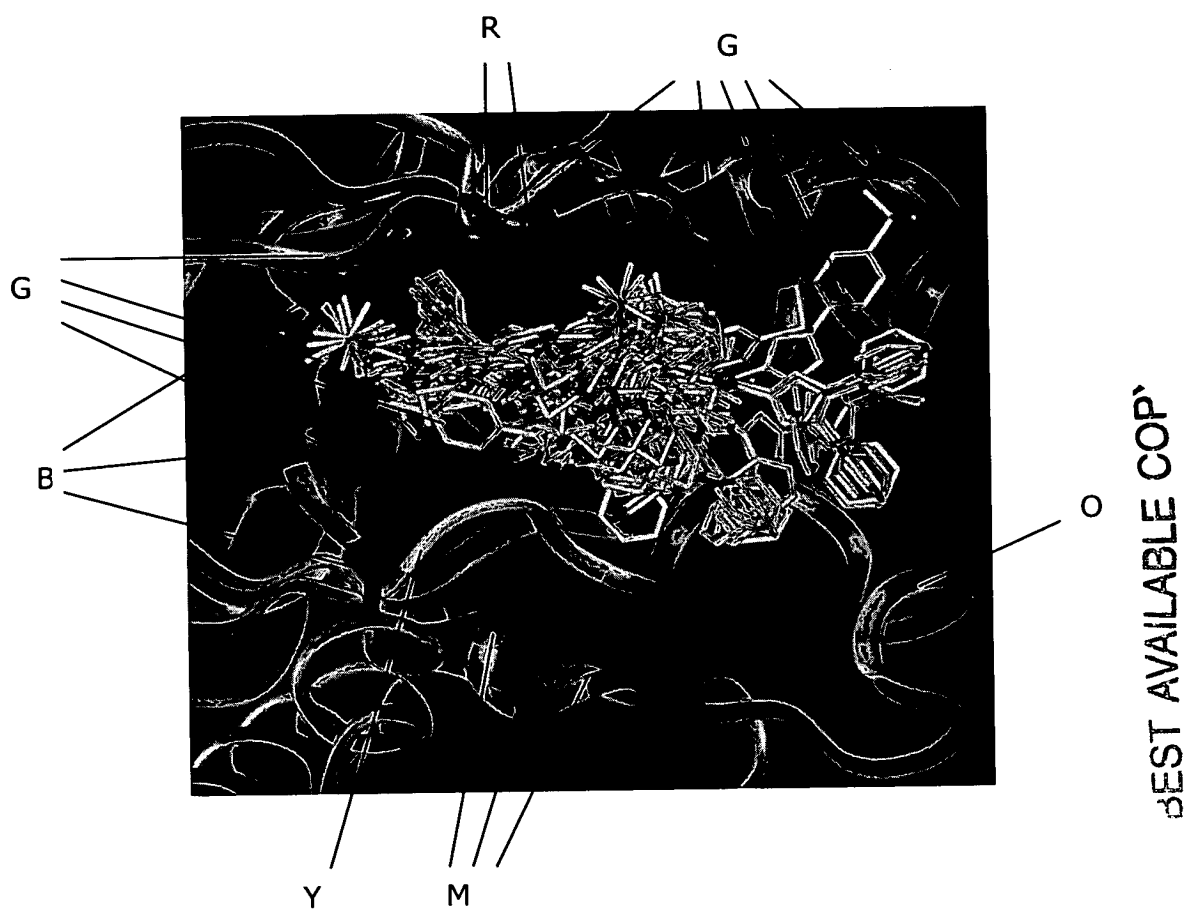


Figure 2A

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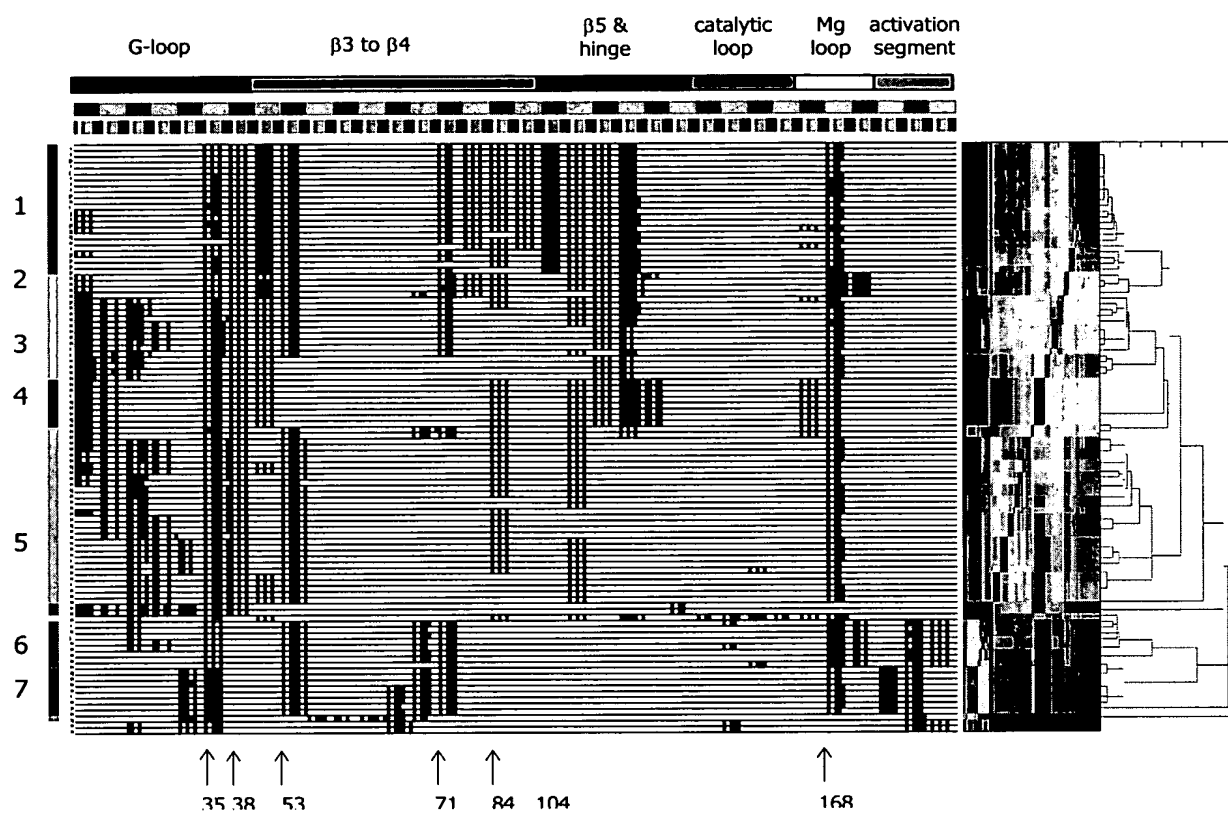


Figure 2B

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Figure 2C

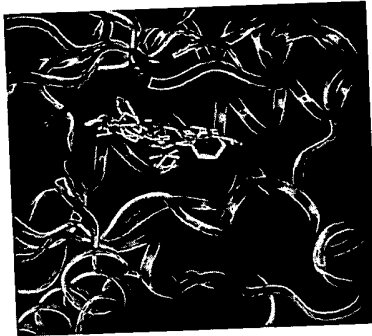


Figure 2D



Figure 2E

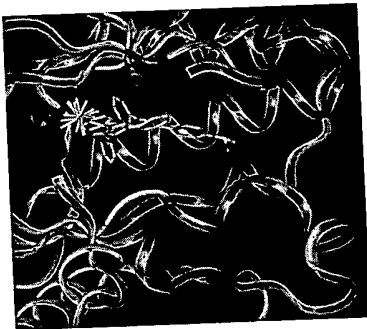


Figure 2F



Figure 2G

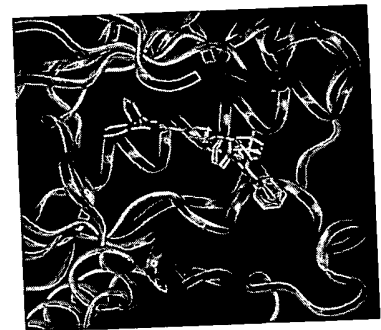


Figure 2H

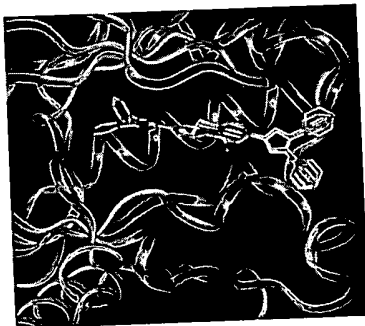


Figure 2I

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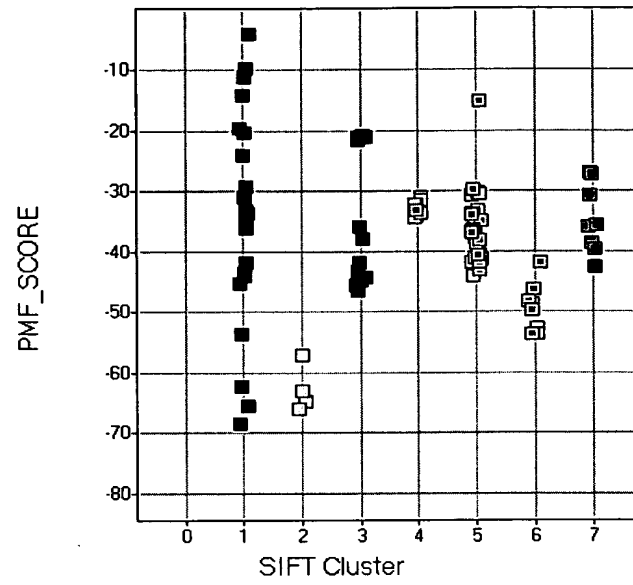


Figure 3A

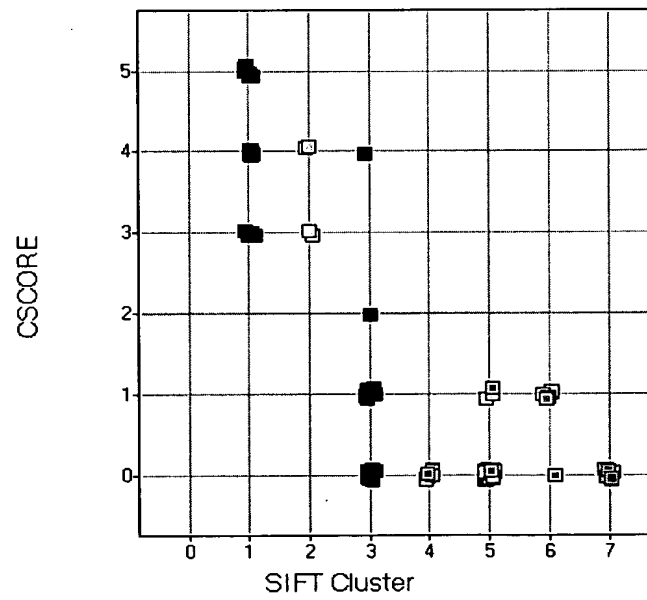


Figure 3B



Figure 4A

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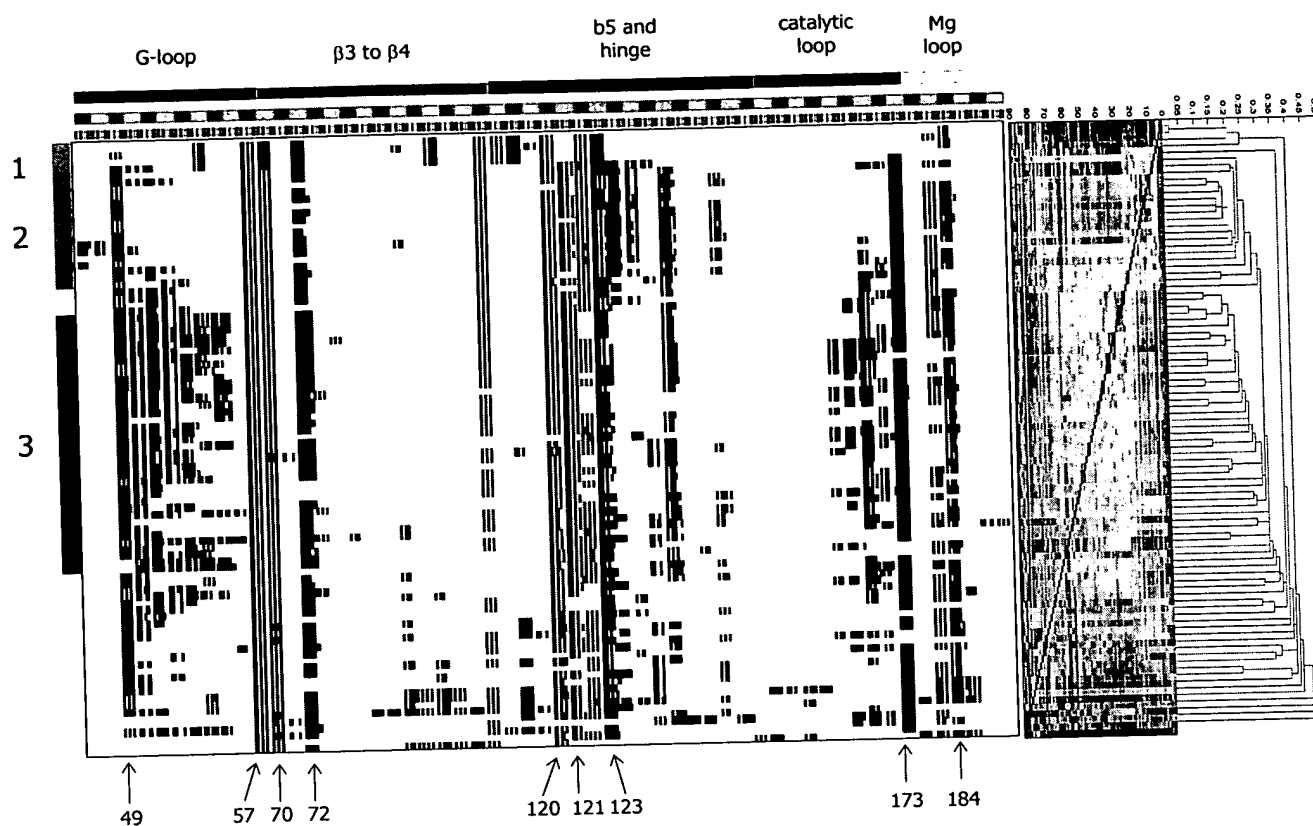


Figure 4B

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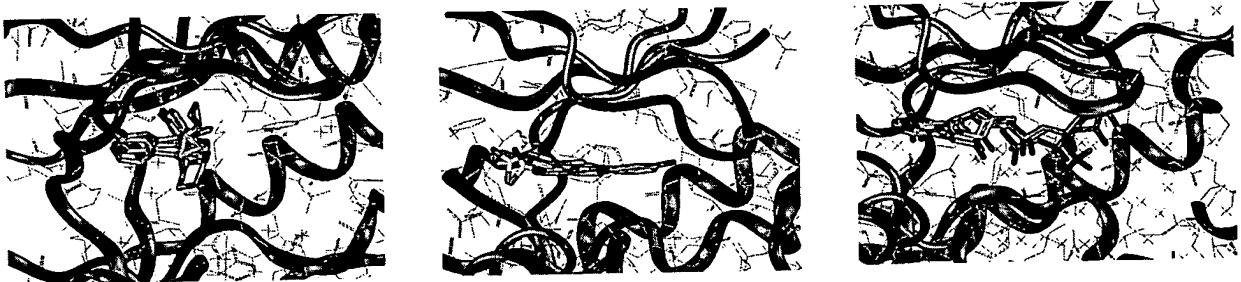


Figure 4C

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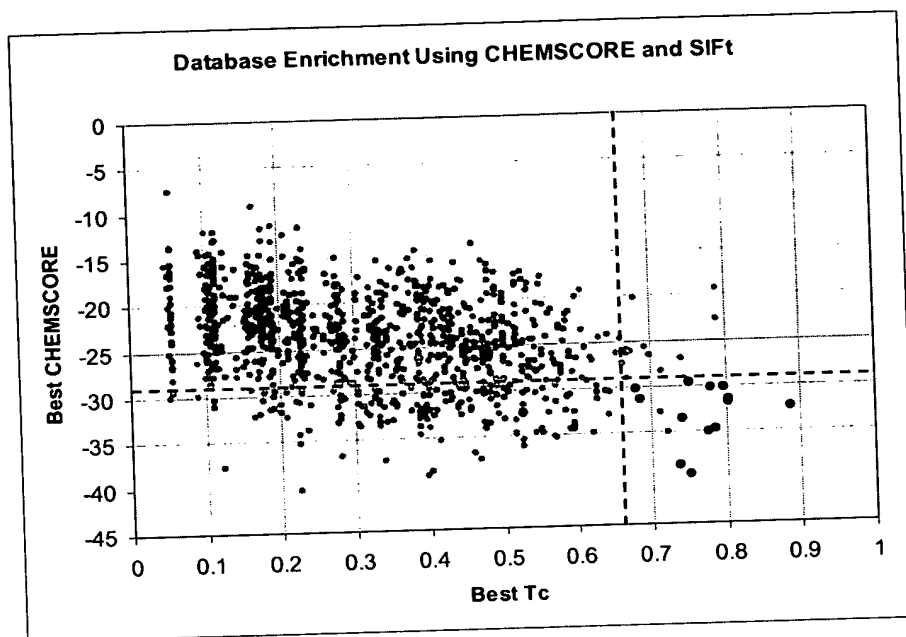


Figure 5A

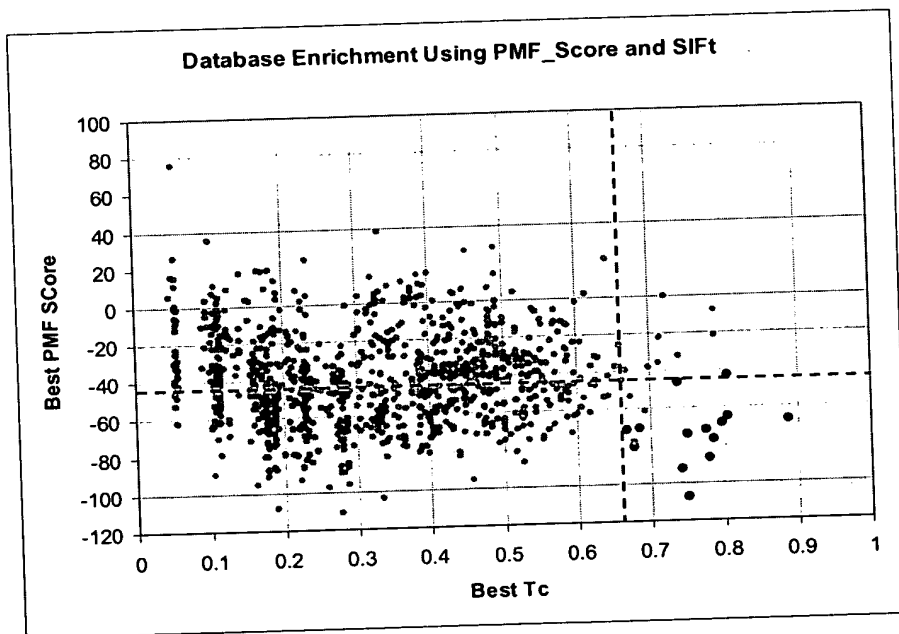
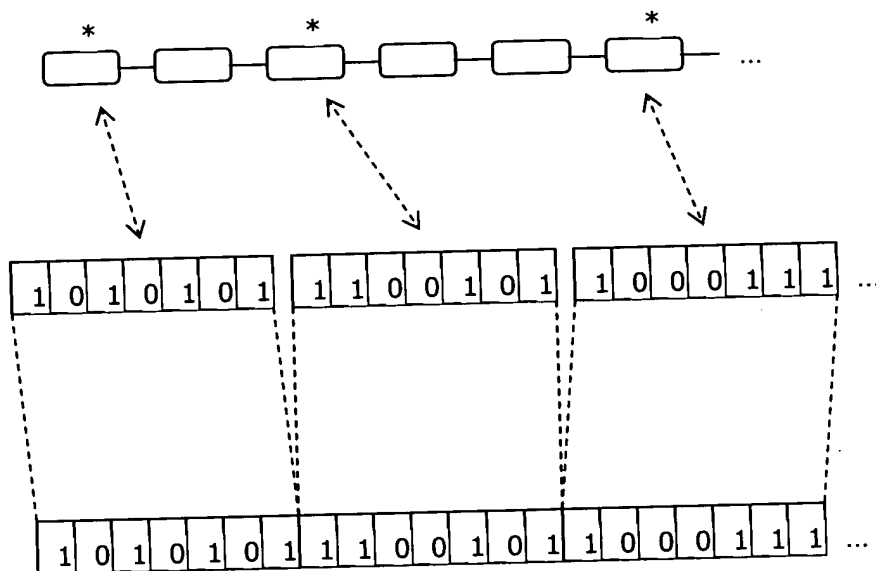
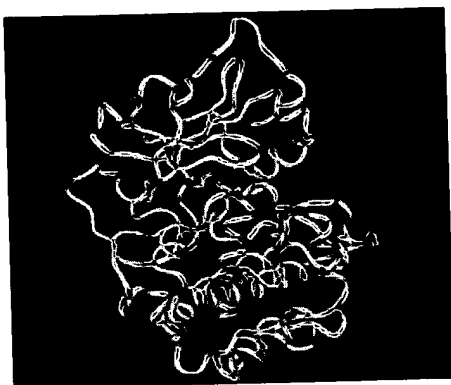


Figure 5B

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Obtain a 3-D structure of a binary complex involved a target molecule and a ligand molecule



Select a plurality of **positions** of interest on the target molecule sequence



Calculate and quantify a plurality of interactions at each position (each block represents an **information block** for the corresponding position; each bit is an **information bit**)



Generate a SIFT by concatenating the information blocks together into a linear **information string**

Figure 6

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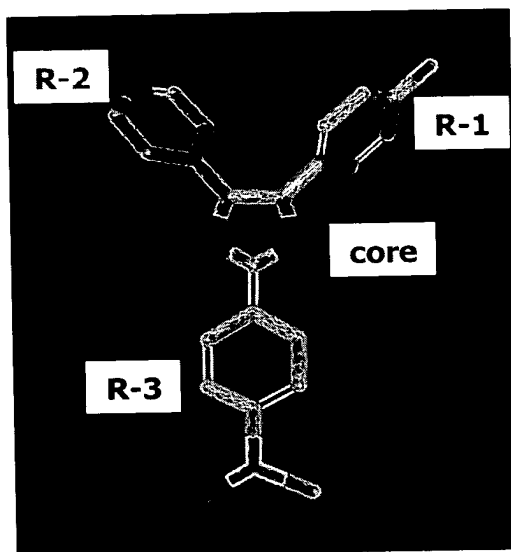


Figure 7A

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(Red: core, Blue: R-3, Yellow: R-2, Green: R-1)

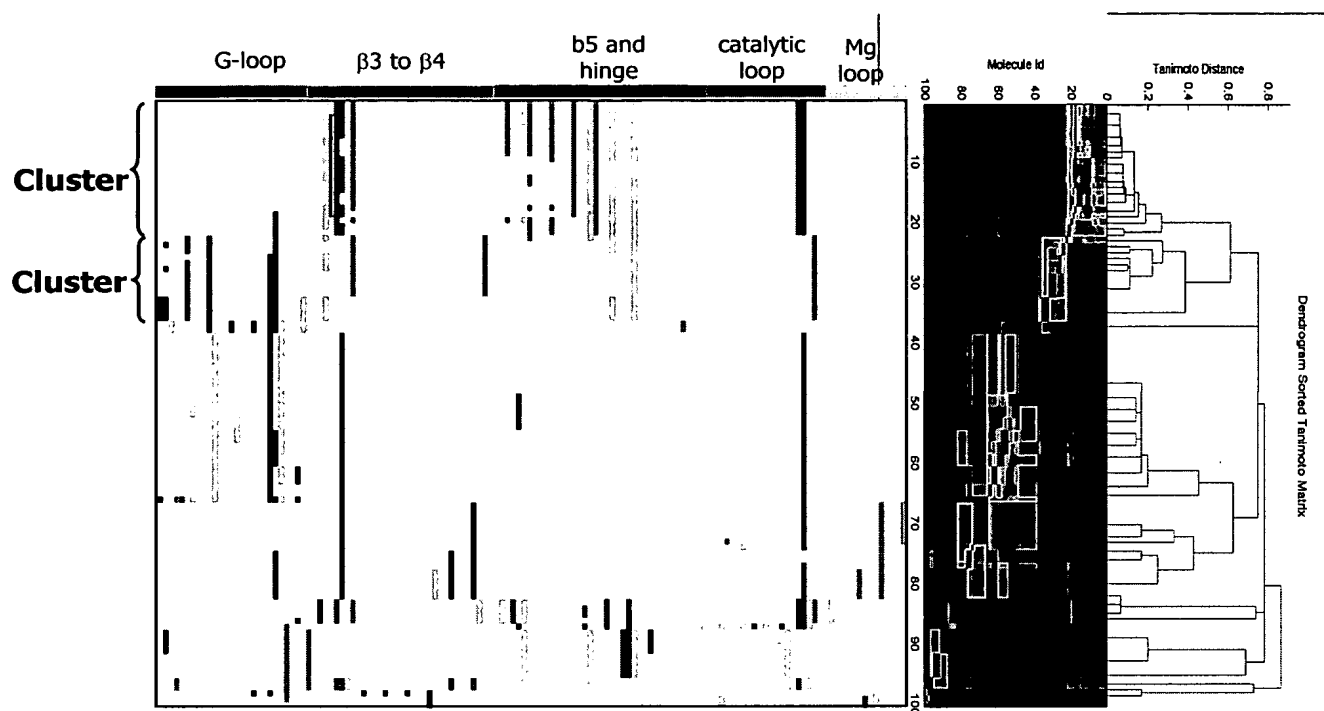


Figure 7B

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Figure 7C

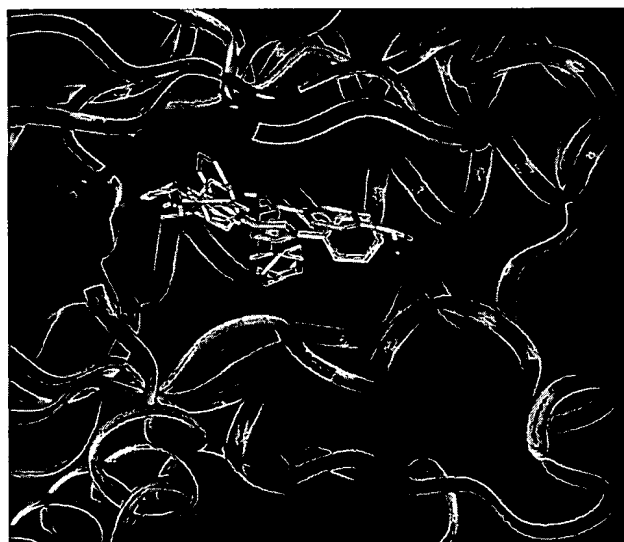


Figure 7C

BEST AVAILABLE COPY

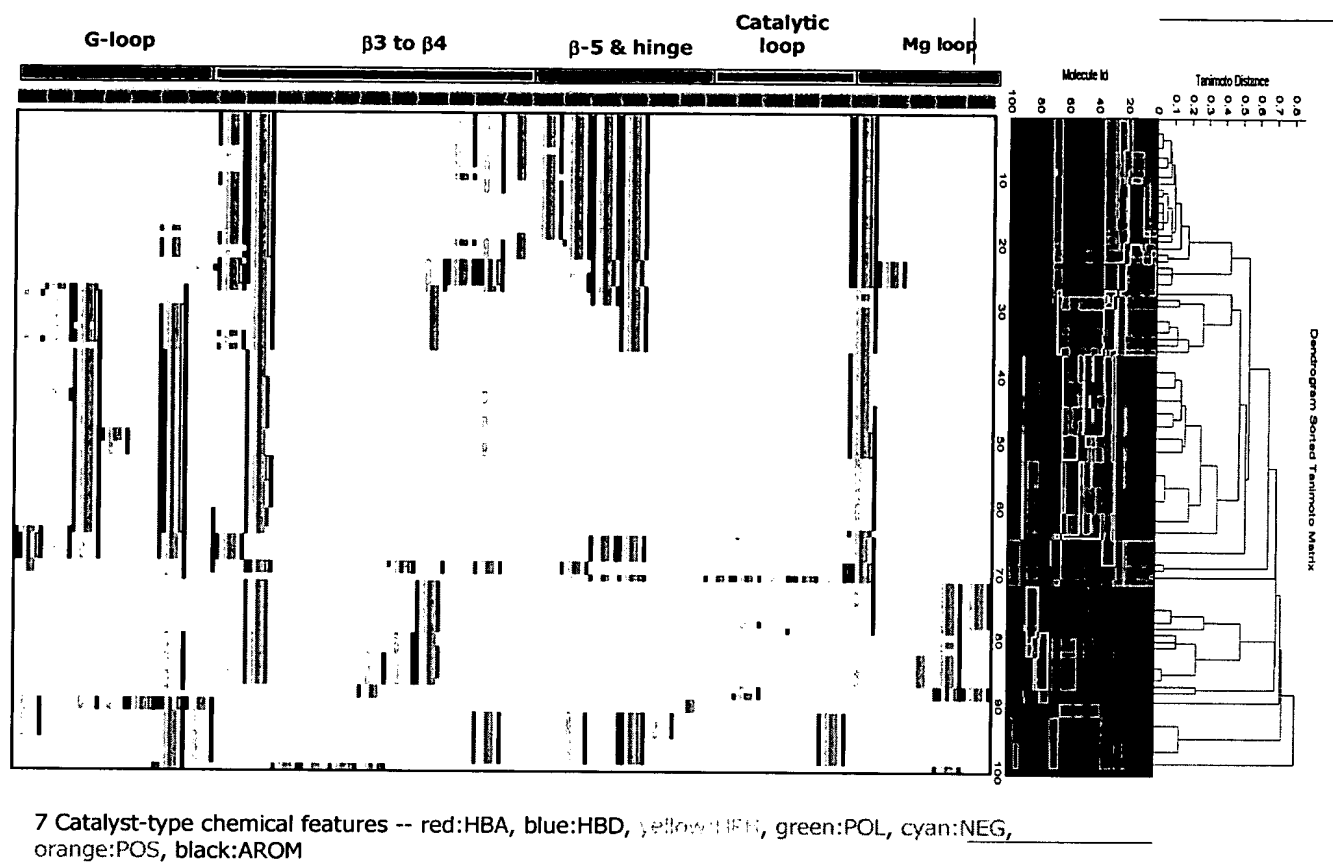


Figure 8

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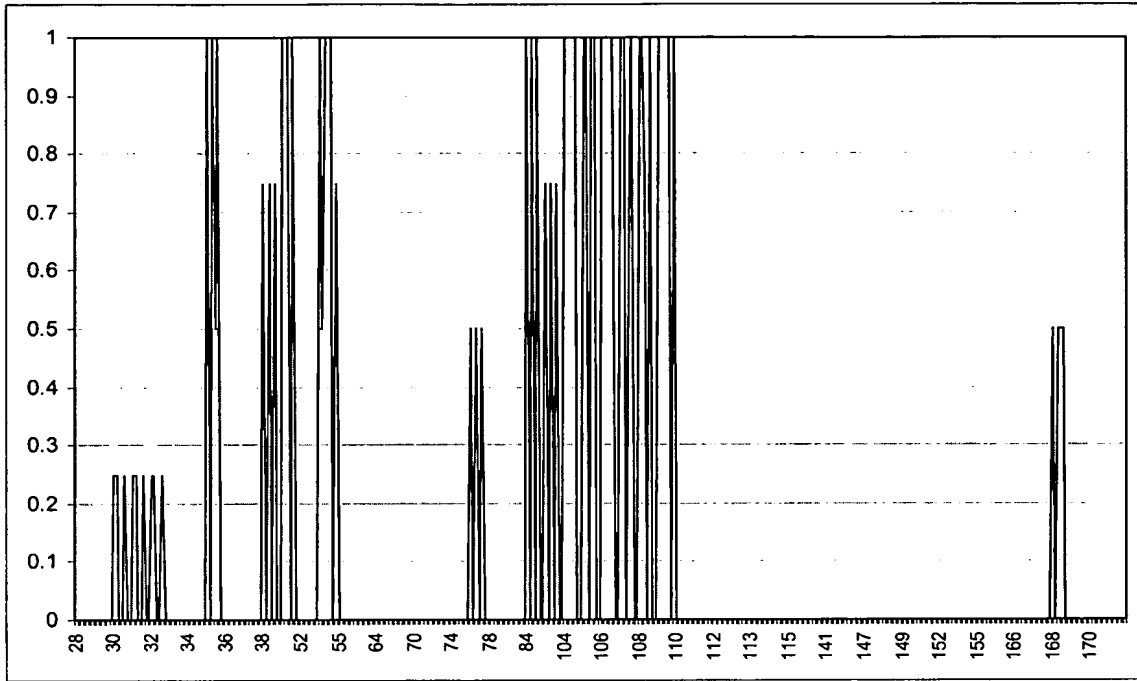


Figure 9A

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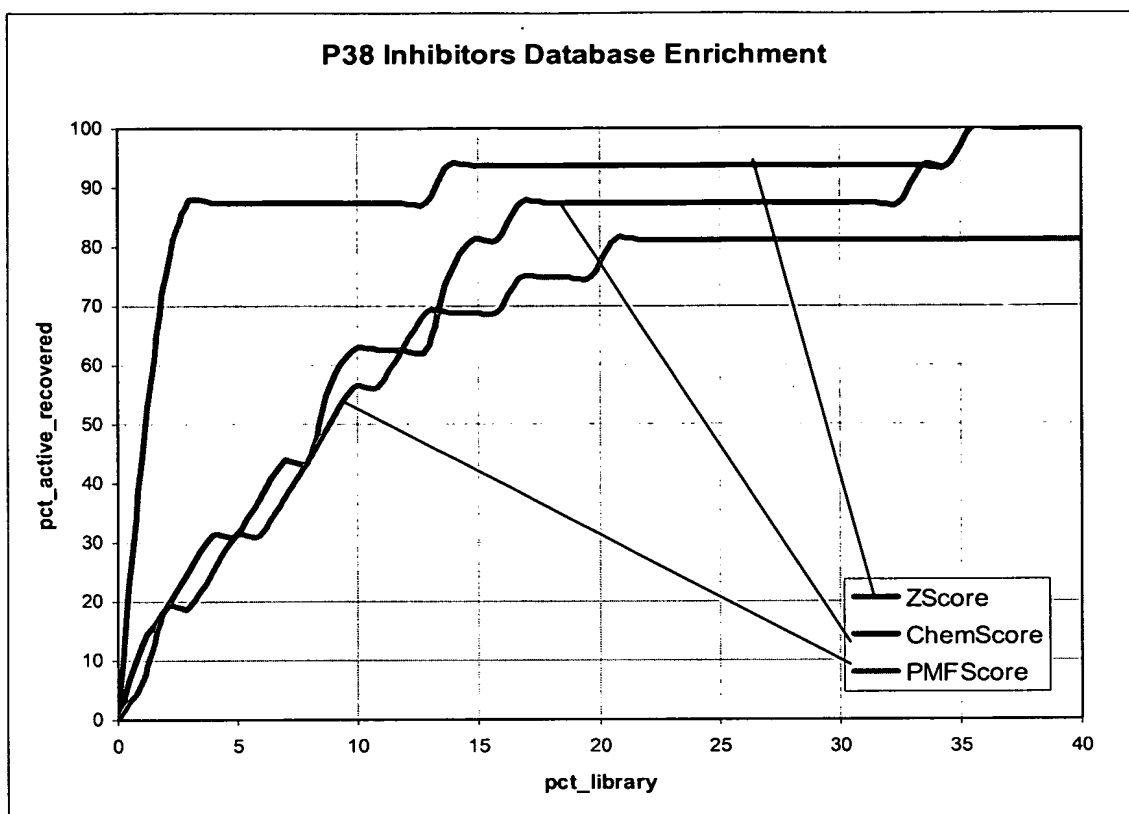


Figure 9B

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